REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
22-09-2016	Final Report	27-Jun-2016 - 26-Jun-2017

4. TITLE AND SUBTITLE	
Final Report: Workshop on quantum stochastic differential equations for the quantum simulation of physical systems	5a. CONTRACT NUMBER W911NF-16-1-0379
	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER 611102
6. AUTHORS George Siopsis	5d. PROJECT NUMBER
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES	8. PERFORMING ORGANIZATION REPORT NUMBER
University of Tennessee at Knoxville Office of Sponsored Programs 1534 White Avenue Knoxville, TN 37996 -1529	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES)	10. SPONSOR/MONITOR'S ACRONYM(S) ARO
U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211	11. SPONSOR/MONITOR'S REPORT NUMBER(S) 69643-MA-CF.1

12. DISTRIBUTION AVAILIBILITY STATEMENT

Approved for Public Release; Distribution Unlimited

13. SUPPLEMENTARY NOTES

The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT

This is a report on the "Workshop on quantum stochastic differential equations for the quantum simulation of physical systems" held at the Adelphi Laboratory Center, Adelphi, MD, on Monday, August 22, 2016. It attracted mathematicians, computer scientists, logicians, and physicists (both theorists and experimentalists) who discussed their research and participated in stimulating discussions on how to apply mathematical tools to the quantum simulation of physical systems of interest to the Army. There were participants from US Government agencies,

15. SUBJECT TERMS

quantum information, quantum systems, quantum probability, quantum topology, quantum field theory, quantum stochastic differential equations, quantum computing

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	c. THIS PAGE	17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
UU	UU	UU	UU		George Siopsis
					19b. TELEPHONE NUMBER 865-974-7846

Report Title

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Report on *"Workshop on quantum stochastic differential equations for the quantum simulation of physical systems"*

George Siopsis

Department of Physics and Astronomy, University of Tennessee, Knoxville, TN

Summary

This is a report on the "Workshop on quantum stochastic differential equations for the quantum simulation of physical systems" held at the Adelphi Laboratory Center, Adelphi, MD, on Monday, August 22, 2016. It attracted mathematicians, computer scientists, logicians, and physicists (both theorists and experimentalists) who discussed their research and participated in stimulating discussions on how to apply mathematical tools to the quantum simulation of physical systems of interest to the Army. There were participants from US Government agencies, industry, and academia. The Workshop was financially supported by ARO via a grant to the University of Tennessee. The web site for the Workshop is http://aesop.phys.utk.edu/QI/Workshop.html.

Participation

Participation was by invitation only. The workshop attracted a diverse set of participants which included mathematicians, computer scientists, logicians, and physicists (both theorists and experimentalists). They came from various US Government agencies (ARL, AFRL, NIST, NSA), industry (IBM), US and Canadian academic institutions (University of Tennessee, University of Waterloo, University of Maryland, Dartmouth College, Northwestern University, MIT, CUNY, Johns Hopkins University).

List of talks

Radhakrishnan Balu (ARL)	*Anatomy of a quantum stochastic differential equation*
George Siopsis (University of Tennessee)	*Quantum simulations with continuous variables*
Raymond Laflamme (Director, Institute for Quantum Computing, University of Waterloo)	*Algorithmic cooling*
Samuel Lomonaco (University of Maryland, Baltimore County)	*Topological Quantum Computation*
David Gosset (Quantum Computing Theory Group, IBM)	*Complexity of quantum impurity models*
Miles Blencowe (Dartmouth College)	*Self-oscillating superconducting circuits, Wigner flows, and the generation of macroscopic quantum states of light*

Jens Koch (Northwestern University)	*Using machine learning to control quantum circuits and produce exotic states of light*
Stephen Jordan (Applied and Computational Mathematics, NIST)	*Quantum Algorithms for Topological Invariants*
Dirk Englund (MIT)	*Quantum Information Processing Using Programmable Silicon Photonic Integrated Circuits*
John Terilla (Queens College, CUNY)	*Homotopy probability theory and fluid flow*
Mohammad Hafezi (University of Maryland, College Park)	*Topological physics in photonics systems*

Army relevance

The various talks at the workshop and the discussions among participants centered around topological quantum field theories (TQFTs), topological quantum information, and simulation of materials with topological properties, as long-term goals of research of interest to the Army. Topological materials are multi-functional materials with very interesting thermal, electronic, and mechanical properties that would be very relevant to DoD applications in general, and Army purposes in particular. Except in special cases, such as graphene, these materials form a whole new class whose potential is yet to be explored. The workshop provided important insights into theoretical and computational efforts to study topological materials that would be complimentary to the efforts at ARL. One the other hand, topological quantum field theories have a dual application to topological quantum computation, which is relevant in the context of the quantum sciences program pursued at ARL. It should also be noted that these quantum systems, by their nature, require the use of mathematical tools of (quantum) probability theory and statistics, along with functional analysis, also of relevance to the mathematics program at ARL.

Discussion

[Workshop participants' names are in **bold** *characters.]*

Quantum simulation was first proposed by Richard Feynman who realized that classical computers could not simulate large physical systems at a microscopic level, because of the enormous amount of data needed to describe the state of such systems. Feynman argued that a quantum system could, instead, efficiently simulate physical systems that would be intractable by classical means (*"Let the computer itself be built of quantum mechanical elements which obey quantum mechanical laws."* [1]). The development of quantum simulators is currently a very active and rapidly growing field of research. Unlike universal quantum computers which can run any conceivable quantum algorithm, quantum simulators are specialized devices that only run quantum algorithms appropriate for a certain physical system (or class of systems). Thus they use fewer resources, and one may be able to build them using existing technology.

Quantum simulators have been based on a variety of architectures, including photons (employed in continuous variable quantum computation, simulation of quantum (stochastic) walks, etc.), neutral atoms, trapped ions, cavity arrays, electronic spins (quantum dots), nuclear spins (NMR), and superconducting circuits. There exist four types of quantum simulation:

1. Digital, which is based on quantum circuits consisting of discrete quantum gates).
2. Analogue, in which one (controllable) quantum system mimics another, and includes adiabatic models.
3. Hybrid, a combination of digital and analogue quantum simulation.
4. Quantum information inspired algorithms for classical simulation.

There is an endless list of applications. To mention a few:

1. Solid state physics (Hubbard and spin models, quantum phase transitions, spin glasses, disordered and frustrated systems, high-temperature superconductors, topological order, etc.).
2. Atomic physics (cavity QED, cooling).
3. Open quantum systems.
4. Chemistry (molecular energies, thermal rates, chemical reactions).
5. Interferometry (Mach-Zehnder, Fano, Fabry-Perot, boson sampling).
6. High energy physics (quantum field theory, Dirac equation, etc.)
7. Relativity and cosmology (Unruh effect, Hawking radiation, Universe expansion).

While quantum mechanics is a deterministic theory defining a unitary time evolution, to extract any physical information one needs to perform a measurement, which involves a stochastic process (collapse of the wavefunction). Thus a full description of a quantum system is provided by a quantum stochastic differential equation (QSDE) [2], introduced at the Workshop by **Balu**. Physical observables yield classical random variables. They are defined as self-adjoint operators on a Hilbert space, themselves forming a Banach space under the operator norm topology. Thus, probability theory and statistics, along with standard tools of functional analysis, can be employed to investigate quantum systems whose dynamics can be naturally captured by quantum analogues of stochastic processes [3]. The mathematical framework for the study of quantum systems is known as quantum (non-commutative) probability theory [4,5]. Important computational tool in the study of open quantum systems are QNET [6], QuTip [7], and QSD [8]. One can use them to derive master equations for the quantum system of interest, and then solve the QSDE numerically [9]. Of particular interest is the development of quantum networks using these tools.

Turning to topological properties of materials, it should be noted that the study of topological invariants has been a fertile ground for interactions between mathematicians and physicists. An important example is the Jones polynomial which is a characteristic polynomial for a knot in three dimensions. Two knots are inequivalent if they have different Jones polynomials. However, the mathematical definition of the Jones polynomial is not manifestly three-dimensional. Witten provided a path-integral definition of the Jones polynomial using a three-dimensional Chern-Simons quantum field theory (QFT) based on a non-abelian gauge field [10]. Even though Witten's expression does not admit a rigorous mathematical definition, it provides an intuitive geometric definition of a topological invariant. The Jones polynomial is also related to other aspects of Mathematical Physics, such as integrable lattice statistical mechanics, and two-dimensional conformal field theory and associated representations of braid groups. A quantum algorithm for computing it was found by **Lomonaco** and Kauffman [11], and was implemented using NMR [12]. At the workshop, **Lomonaco** discussed a research program based on quantum knots developed by him and Kauffman [13,14] which can be useful in robust quantum information processing.

Knot invariants and a quantum algorithm for the Jones polynomial were also discussed at the Workshop by **Jordan**. He and Shor have shown that Jones polynomials can be approximated in time which is polynomial in both the number of strands and number of crossings by quantum computation in which all but one qubit start in the maximally mixed state (one clean qubit model) [15]. Moreover, the problem of simulating a one-clean-qubit computer is reducible to a certain approximation of the Jones polynomial at the fifth root of unity for the trace closure of a braid. Thus, the latter is a complete problem for the one-clean-qubit complexity class. This has been experimentally verified by Passante, Moussa, Ryan, and **Laflamme** [16], as well as Marx, Kauffman, **Lomonaco**, Spörl, Pomplun, Schulte-Herbrüggen, Myers, and Glaser [17]. **Jordan** and collaborators also established a relation between the task of distinguishing non-homeomorphic three-manifolds and the power of a quantum computer by showing that approximating certain Turaev-Viro invariants (scalar topological invariants of compact, orientable three-manifolds) presented by Heegaard splittings is a universal problem for quantum computation [18]. Subsequently, **Jordan** and Alagic extended these results by showing that the problem of estimating the Fibonacci version of the Turaev-Viro invariant of a mapping torus is a complete problem for the one-clean-qubit complexity class [19]. This study in topological quantum information provides insights in pure mathematics, such as the solutions to the Yang-Baxter equations [20]. It is also important for the simulation of physical systems, such as the quantum Hall effect.

TQFTs possessing a gauge symmetry provide an intuitive physical arena in which one can study topological invariants. While gauge theories are ubiquitous in a physicist's arsenal, mathematical concepts are governed by formal logic as they are constructed from a foundational set of axioms, such as set theory or type theory. The latter is in fact well-suited for verification of formal mathematics by a computer. It is a challenge to apply computer-based verification of TQFTs and, more generally, quantum gauge field theories, because of their complexity. Recent progress has been achieved via Cohesive Homotopy Type Theory [21,22]. It was shown that it serves as a formal foundation for central concepts in quantum gauge field theories. This points to the interesting possibility of applying automated proof-checkers on various concepts in TQFTs, which is worth exploring. This was pointed out at the Workshop by **Balu** and **Terilla**. As **Terilla** remarked, homotopy theory captures and repackages QFT tools for other fields, such as probability theory and the study of fluid flow via the Euler equation [23].

An important physical realization of quantum systems is provided by continuous variables (CVs) based primarily on photonic systems, as discussed at the Workshop by **Siopsis**. CVs offer the exciting possibility of realizing quantum information processing with existing technology. In addition to Gaussian gates which have already been implemented, one needs to construct a non-Gaussian element (gate). Such gates have been proposed using the GKP scheme [24], the MFF scheme [25], and by **Siopsis** and collaborators [26]. The last one was used in an algorithm to simulate scattering amplitudes in QFT [27], which had certain advantages over its discrete-variable (DV) counterpart introduced by **Jordan**, Lee, and Preskill [28,29], as well as algorithms for quantum machine learning [30] to be compared with their DV counterparts [31,32]. A central ingredient is the exponential swap gate [33] whose physical implementation was discussed in the Workshop by **Hafezi**. For practical applications, one needs to perform quantum error correction which is still in its infancy for CV systems. Even though non-Gaussian errors need only Gaussian elements to correct [34,35], Gaussian error correction requires the use of non-Gaussian elements [36]. Moreover, algorithms require the use of eigenstates of quadrature operators which can only be approximately physically realized as squeezed states. Information is encoded on cat states (superpositions of coherent states) [24,37]. They can be shown to be robust against errors through implementation within circuit QED using QSDEs [38]. In general, they need to obey Knill-**Laflamme** conditions [39]. A promising alternative is a quantum error suppression scheme, such as dynamical decoupling (bang-bang control) [40,41], which has already been successfully applied to nuclear spin systems [42], photonic qubits [43], and DV quantum computing [44]. It would be interesting to explore the possibility of applying it for error suppression in CV quantum information processing.

Quantum error correction was further discussed at the Workshop by **Laflamme**. He concentrated on algorithmic cooling in an ensemble setting (solid-state NMR at low polarization) which provides a way to remove entropy from the system. Algorithmic cooling can be improved using a heat bath. **Laflamme** and collaborators recently analyzed the control of the relaxation dynamics of a two-qubit NMR spin system [45]. They followed a numerical approach, approximately computing the reachable set of states for coherently controlled quantum Markovian systems. The approximation consisted of setting both upper and lower bounds for system's reachable region of states. By implementing certain experimental tasks of quantum state engineering in this open system at a near optimal performance in view of purity (e.g., increasing polarization, and preparing pseudopure states), they demonstrated the usefulness of their approach and showed interesting and promising applications of environment-assisted quantum dynamics. Precisely characterizing and controlling realistic quantum systems under noise is a challenging frontier in quantum science and technology. In developing reliable controls for open quantum systems, one is often confronted with the problem of the lack of knowledge on the system controllability. Developing quantum control methods and solving the resulting QSDEs is an active area of research.

The use of photonic systems in the simulation of topological properties of physical systems were discussed at the Workshop by **Hafezi** from an experimental point of view. He and collaborators have shown how photonic devices can be improved by exploiting topological properties of optical systems. They demonstrated how quantum spin Hall Hamiltonians can be created with linear optical elements using a network of coupled resonator optical waveguides in two dimensions. They found that key features of quantum Hall systems, including the characteristic Hofstadter butterfly and robust edge state transport, can be obtained in such systems. As an application, they showed that topological protection can be used to improve the performance of optical delay lines and to overcome some limitations related to disorder in photonic technologies [46]. **Hafezi** and collaborators also realized synthetic magnetic fields for photons at room temperature using linear silicon photonics, and observed topological edge states of light in a two-dimensional system which were robust against intrinsic and introduced disorder. Their experiment demonstrated the feasibility of using photonics to realize topological order in both non-interacting and many-body regimes [47,48]. The exploration of topological properties of light is an active field of research [49-59]. Notable applications are in the fractional quantum Hall effect [60] and confined topological edge states in photonic crystals [61].

The simulation of physical systems from an experimental point of view using photonic integrated circuits was discussed at the Workshop by **Englund**. He and collaborators have shown that existing fabrication processes are sufficient to build quantum photonic processors that are capable of high-fidelity operation

[62]. They proposed and analyzed the design of a programmable photonic integrated circuit for high-fidelity quantum computation and simulation. They demonstrated that the reconfigurability of their design allowed them to overcome some major impediments to quantum optics on a chip. They also simulated an experiment enabled by the programmability of their system for a statistically robust study of the evolution of entangled photons in disordered quantum walks. **Englund** also discussed schemes for an efficient architecture of linear optics experiments by using, e.g., time-bin encoding and dispersive optics based unitary transformations [63], and all-optical quantum repeaters [64,65].

Koch discussed the application of QSDEs to machine learning for controlling quantum circuits and producing exotic states of light. Systems of interest are described by QFT and simulated on a lattice which must include driving and dissipation (open quantum lattice, such as the open Jaynes-Cummings lattice) [66]. An important requirement for a large-scale quantum information processor is the ability to construct control pulses to implement an arbitrary quantum circuit in a scalable manner. An analysis of errors in control imperfections in a liquid-state NMR system was performed by **Laflamme** and collaborators [67]. As engineered quantum systems become increasingly complex, machine learning (closed loop control) can become an efficient tool, especially in open systems with topological protection.

Gosset discussed quantum impurity models which provide a powerful numerical method for calculating electronic structure of strongly correlated materials such as transition metal compounds and high-temperature superconductors. These materials are described by a fermionic lattice QFT and can be studied using impurity models within the dynamical mean field theory approximation. Bravyi and Gosset used mathematical tools for a fast estimation of the ground state and low energy states of quantum impurity models [68]. These results may be useful in hybrid quantum-classical simulations of correlated materials.

Blencowe discussed how to engineer strongly nonlinear, superconducting circuit devices that can continuously generate macroscopic quantum states of light (non-classical microwaves involving large average photon number). He and collaborators investigated the quantum versus classical dynamics of a microwave cavity-coupled-Cooper pair transistor system, where an applied dc bias causes the system to self-oscillate via the ac Josephson effect [69]. The QSDE governing the system exhibits such phenomena as dynamical tunneling and the generation of non-classical states from initial classical states. The system may be capable of demonstrating macroscopic quantum dynamical behavior, obviating the need for an external ac-drive line, which typically is harder to noise filter than a dc bias line. **Blencowe**, *et al*., also studied the quantum dynamics of a model circuit consisting of a voltage-biased Josephson junction and a superconducting cavity, focusing on the (nonlinear) regime where a single cavity mode is strongly excited. The system exhibited quadrature and amplitude squeezing over a broad range of parameters [70]. It would be interesting to understand further how classical nonlinearities generate corresponding non-classical states [71,72], and generalize the results to many-body systems. Wigner flow may be a useful tool for elucidating how non-classical states are generated by nonlinearities and destroyed by noise. It would be interesting to exploit Wigner flow and other tools for developing an understanding of how to engineer strongly nonlinear, self-oscillating superconducting circuit devices as tunable, continuous non-classical microwave sources. The theoretical challenge is to determine the steady cavity quantum state, given large Q (long relaxation time), and large photon number (large Hilbert space dimension).

Conclusion

This was a successful Workshop that attracted leading researchers from across the US and Canada who engaged in stimulating discussions. The state of the art of mathematical tools, such as quantum stochastic differential equations, which are necessary for the development of quantum simulators was discussed at the Workshop. The main focus was on topological quantum field theories, topological quantum information, and simulation of materials with topological properties. Discussions among participants centered around novel mathematical tools and approximation schemes that are needed in order to further develop our understanding of physical systems off equilibrium, large ensembles, and strong correlations and couplings. The discussions involved a synergy between mathematicians and other theorists, as well as experimentalists who can take advantage of mathematical tools, and provide feedback regarding the physical realization of mathematical tools. The Workshop was an important event toward the advancement of research in the field, and a milestone as ARL becomes a significant player in the development of mathematical tools for quantum systems of interest to the Army.

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